Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(2-furylmethylene)-1,1′-binaphthyl-2,2′-diamine

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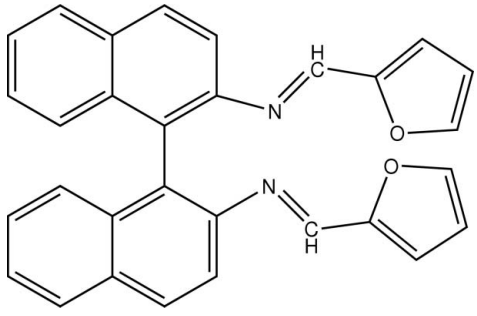
Received 22 November 2007; accepted 5 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.062; wR factor = 0.146; data-to-parameter ratio = 12.1.

In the title compound, $C_{30}H_{20}N_2O_2$, the orientation of the furyl group may induce a variety of coordination modes with this ligand. The dihedral angle between the two naphthyl rings is 79.25 (7)°. The furyl groups make dihedral angles of 62.0 (1) and 16.3 (2)° with the attached naphthyl groups. The dihedral angle between the two furyl rings is 49.3 (2)°.

Related literature

For related literature see: Chen *et al.* (1995); Dang *et al.* (1971); Grubbs *et al.* (1977); Horner *et al.* (1968); Miyashita *et al.* (1980); Nishinaga *et al.* (1988); Pertici *et al.* (1996); Rosini *et al.* (1992); Suda *et al.* (1983); Spassky *et al.* (1996); Suga *et al.* (2003).



Experimental

Crystal data

$C_{30}H_{20}N_2O_2$
M_r = 440.48
Monoclinic, $P2_1/n$
a = 8.2433 (2) Å
b = 15.5046 (3) Å
c = 17.7432 (3) Å
β = 91.309 (3)°
V = 2267.15 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.23 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: none
4133 measured reflections
4016 independent reflections
1600 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
2 standard reflections
frequency: 120 min
intensity decay: −1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.146
S = 0.97
4016 reflections
331 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ2001).

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 doi:10.1107/S1600536807065750

supplementary materials

Acta Cryst. (2008). E**64**, o271 [**doi:10.1107/S1600536807065750**]

N,*N*'-Bis(2-furylmethylene)-1,1'-binaphthyl-2,2'-diamine

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Comment

The importance of axially chiral ligands in catalytic asymmetric reactions is well known in the development of stereoselective hydrogenation of olefins·The low enantiomeric excess induced by the first chiral monodentate phosphane ligands (Horner *et al.*, 1968) was soon enhanced by chelating bisphosphanes (Dang *et al.*, 1971). Axially chiral ligands were first reported in a hydrogenation reaction in 1977 and have gained ground ever since (Grubbs *et al.*, 1977)·In addition to the biaryl backbone bisphosphanes (2,2'-bis (diphenylphosphino)-1,1'-binaphthyl) (Miyashita *et al.*, 1980), derivatives of the corresponding diamines (biphenyldiamine and binaphthyldiamine) have performed successfully in many asymmetric catalytic reactions (Rosini *et al.*, 1992). These include stereoselective polymerizations of methacrylate (Suda *et al.*, 1983) and lactate (Spassky *et al.*, 1996) and numerous enantioselective modifications of olefins such as epoxidation (Nishinaga *et al.*, 1988), aziridination (Suga *et al.*, 2003), cyclopropanation (Chen *et al.*, 1995) and hydrogenation (Pertici *et al.*, 1996). With a structurally rigid binaphthyl ligand backbone, the configuration of the ligand is fixed and its axial chirality can efficiently be transmitted to the active site catalyst. We report here the crystal structure of (I) which was synthesized *via* condensation of the axially chiral binaphthyldiamine with the 2-furfuraldehyde. The centrosymmetric crystal structure shows that there is racemization which may occur during the reaction of condensation. The molecule of (I) has two imine groups with bond distances N1—C1 1.264 (5) Å and N2—C26 1.268 (4) Å. Each imine group is bound to a furfuryl group such that C1—C2 1.445 (5) and C26—C27 1.431 (5) Å. Variation between N—C (N1—C1 and N2—C26) and C—C (C1—C2 and C26—C27) bonds are statistically insignificant. The naphthyl rings make a dihedral angle of 79.25 (7) ° with one another. The furyl group C2C3C4C5O1 makes a dihedral angle of 62.0 (1) ° with its attached binaphthyl group. The other furyl makes a dihedral angle of 16.3 (2) ° with its binaphthyl group. The furyl groups make a dihedral angle of 49.3 (2) ° with one another.

Experimental

The title compound was obtained as follows: to a stirred solution of the 2-furfuraldehyde (0.067 g, 0.703 mmol) in absolute ethanol (10 ml) was added the enantiomerically pure 2,2'-diamino-1,1'-binaphthyl (0.1 g,0.35 mmol). The resulting suspension was heated at reflux for 24 h. The pure yellow ligand was obtained after crystallization in absolute ethanol.

Refinement

Hydrogen atoms H1, H3, H4, H5, H26, H28, H29 and H30 were located in a Fourier map and refined freely. All the other H atoms were placed in calculated positions and allowed to ride during subsequent refinement. The range of bond lengths to hydrogen is between 0.92 and 1.09 Å. U_{iso} of the H atoms were set to be equal to 1.2 U_{iso} of the parent atoms.

Figures

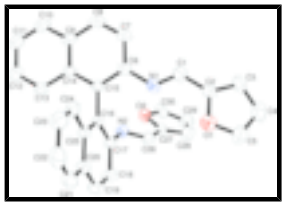


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted.

N,*N*'-Bis(2-furylmethylene)-1,1'-binaphthyl-2,2'-diamine

Crystal data

$C_{30}H_{20}N_2O_2$	F_{000} = 920
M_r = 440.48	D_x = 1.290 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 8.2433 (2) Å	θ = 9.9–11.0º
b = 15.5046 (3) Å	μ = 0.08 mm^{-1}
c = 17.7432 (3) Å	T = 293 (2) K
β = 91.309 (3)º	Prism, yellow
V = 2267.15 (8) Å^3	0.23 × 0.15 × 0.12 mm
Z = 4	

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.028
Radiation source: fine-focus sealed tube	θ_{max} = 25º
Monochromator: graphite	θ_{min} = 2.3º
T = 293(2) K	h = −10→10
non–profiled ω scans	k = 0→18
Absorption correction: none	l = 0→21
4133 measured reflections	2 standard reflections
4016 independent reflections	every 120 min
1600 reflections with $I > 2\sigma(I)$	intensity decay: −1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.146	$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.97	$(\Delta/\sigma)_{max} < 0.001$

4016 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
331 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.9295 (4)	0.7193 (2)	−0.20480 (18)	0.0883 (10)
O2	0.4942 (3)	0.94701 (19)	−0.06519 (15)	0.0583 (7)
N1	1.0080 (4)	0.7947 (2)	−0.0674 (2)	0.0614 (10)
N2	0.6396 (3)	0.7971 (2)	−0.00840 (18)	0.0503 (9)
C1	1.0368 (5)	0.8348 (3)	−0.1278 (3)	0.0640 (13)
H1	1.086 (4)	0.900 (2)	−0.128 (2)	0.077*
C2	1.0049 (5)	0.7968 (3)	−0.2010 (3)	0.0572 (11)
C3	1.0277 (6)	0.8265 (3)	−0.2713 (3)	0.0731 (15)
H3	1.068 (5)	0.882 (3)	−0.281 (2)	0.088*
C4	0.9647 (6)	0.7628 (4)	−0.3211 (3)	0.0820 (16)
H4	0.959 (5)	0.767 (3)	−0.373 (2)	0.098*
C5	0.9084 (6)	0.7002 (4)	−0.2798 (3)	0.0917 (17)
H5	0.863 (5)	0.635 (3)	−0.284 (2)	0.110*
C6	1.0290 (4)	0.8361 (2)	0.0035 (2)	0.0510 (11)
C7	1.1278 (5)	0.9100 (3)	0.0148 (3)	0.0685 (13)
H7	1.1838	0.9331	−0.0254	0.082*
C8	1.1413 (5)	0.9477 (3)	0.0842 (3)	0.0670 (12)
H8	1.2056	0.9965	0.0908	0.080*
C9	1.0583 (5)	0.9130 (3)	0.1462 (3)	0.0530 (11)
C10	1.0706 (5)	0.9520 (3)	0.2183 (3)	0.0677 (13)
H10	1.1338	1.0012	0.2252	0.081*
C11	0.9906 (6)	0.9180 (3)	0.2772 (3)	0.0758 (14)
H11	1.0008	0.9432	0.3247	0.091*
C12	0.8931 (5)	0.8453 (3)	0.2669 (2)	0.0688 (13)
H12	0.8363	0.8233	0.3073	0.083*
C13	0.8799 (5)	0.8062 (3)	0.1986 (2)	0.0568 (11)
H13	0.8159	0.7571	0.1930	0.068*
C14	0.9628 (4)	0.8395 (2)	0.1355 (2)	0.0461 (10)

C15	0.9504 (4)	0.7992 (2)	0.0629 (2)	0.0440 (10)
C16	0.8575 (4)	0.7176 (2)	0.05238 (19)	0.0417 (9)
C17	0.7078 (4)	0.7177 (3)	0.0167 (2)	0.0475 (10)
C18	0.6187 (5)	0.6405 (3)	0.0082 (2)	0.0637 (12)
H18	0.5171	0.6412	−0.0156	0.076*
C19	0.6821 (5)	0.5652 (3)	0.0349 (2)	0.0703 (13)
H19	0.6199	0.5152	0.0309	0.085*
C20	0.8384 (5)	0.5600 (3)	0.0684 (2)	0.0585 (11)
C21	0.9119 (7)	0.4816 (3)	0.0909 (2)	0.0769 (14)
H21	0.8541	0.4303	0.0859	0.092*
C22	1.0659 (7)	0.4800 (3)	0.1198 (3)	0.0835 (16)
H22	1.1131	0.4280	0.1346	0.100*
C23	1.1524 (6)	0.5562 (3)	0.1273 (2)	0.0754 (14)
H23	1.2581	0.5548	0.1467	0.090*
C24	1.0856 (5)	0.6329 (3)	0.1068 (2)	0.0610 (12)
H24	1.1461	0.6831	0.1129	0.073*
C25	0.9267 (5)	0.6381 (2)	0.0765 (2)	0.0472 (10)
C26	0.5987 (5)	0.8037 (3)	−0.0775 (2)	0.0540 (11)
H26	0.619 (4)	0.759 (2)	−0.1130 (19)	0.065*
C27	0.5253 (5)	0.8786 (3)	−0.1108 (2)	0.0525 (11)
C28	0.4798 (7)	0.8988 (3)	−0.1816 (3)	0.0823 (16)
H28	0.500 (5)	0.863 (3)	−0.223 (2)	0.099*
C29	0.4167 (6)	0.9820 (4)	−0.1811 (3)	0.0842 (17)
H29	0.370 (5)	1.015 (3)	−0.221 (2)	0.102*
C30	0.4264 (6)	1.0095 (3)	−0.1108 (3)	0.0713 (14)
H30	0.399 (5)	1.066 (2)	−0.082 (2)	0.085*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C15	0.039 (2)	0.042 (2)	0.050 (3)	−0.0070 (19)	−0.009 (2)	0.006 (2)
O2	0.0567 (17)	0.0603 (19)	0.0581 (17)	0.0050 (16)	0.0043 (14)	0.0058 (17)
C14	0.037 (2)	0.044 (3)	0.056 (3)	−0.004 (2)	−0.013 (2)	0.004 (2)
N2	0.0426 (19)	0.057 (2)	0.051 (2)	−0.0002 (17)	−0.0076 (17)	−0.0008 (18)
C16	0.043 (2)	0.041 (2)	0.041 (2)	−0.005 (2)	−0.0010 (18)	0.0004 (19)
C6	0.048 (3)	0.047 (3)	0.058 (3)	−0.004 (2)	−0.002 (2)	0.003 (2)
C17	0.046 (2)	0.047 (3)	0.049 (3)	−0.004 (2)	−0.006 (2)	0.000 (2)
N1	0.065 (2)	0.065 (2)	0.055 (2)	−0.013 (2)	0.0055 (19)	0.011 (2)
O1	0.104 (3)	0.089 (3)	0.073 (2)	−0.031 (2)	0.0025 (19)	0.001 (2)
C9	0.045 (3)	0.045 (3)	0.068 (3)	−0.004 (2)	−0.014 (2)	−0.002 (2)
C18	0.058 (3)	0.053 (3)	0.079 (3)	−0.011 (3)	−0.014 (2)	−0.009 (2)
C27	0.055 (3)	0.055 (3)	0.047 (3)	−0.008 (2)	−0.009 (2)	0.007 (2)
C12	0.080 (3)	0.073 (3)	0.053 (3)	−0.006 (3)	−0.005 (2)	−0.010 (3)
C25	0.055 (3)	0.043 (3)	0.044 (2)	−0.006 (2)	−0.001 (2)	0.000 (2)
C2	0.056 (3)	0.050 (3)	0.066 (3)	−0.002 (2)	0.009 (2)	0.007 (3)
C26	0.049 (3)	0.059 (3)	0.053 (3)	−0.005 (2)	−0.003 (2)	−0.009 (2)
C20	0.068 (3)	0.053 (3)	0.055 (3)	−0.009 (3)	0.001 (2)	0.002 (2)
C8	0.051 (3)	0.056 (3)	0.094 (4)	−0.015 (2)	−0.007 (3)	−0.008 (3)

C13	0.062 (3)	0.051 (3)	0.057 (3)	−0.008 (2)	−0.007 (2)	0.000 (2)
C24	0.068 (3)	0.055 (3)	0.059 (3)	0.006 (2)	−0.016 (2)	0.005 (2)
C1	0.071 (3)	0.055 (3)	0.066 (3)	0.001 (3)	0.010 (3)	−0.005 (3)
C7	0.059 (3)	0.063 (3)	0.084 (4)	−0.021 (2)	0.007 (3)	0.005 (3)
C30	0.066 (3)	0.067 (3)	0.081 (4)	0.005 (3)	0.009 (3)	0.024 (3)
C11	0.089 (4)	0.072 (4)	0.065 (3)	−0.002 (3)	−0.019 (3)	−0.015 (3)
C10	0.067 (3)	0.051 (3)	0.084 (3)	−0.009 (2)	−0.024 (3)	−0.011 (3)
C21	0.117 (4)	0.049 (3)	0.065 (3)	−0.003 (3)	0.004 (3)	0.009 (2)
C23	0.085 (3)	0.064 (3)	0.076 (3)	0.010 (3)	−0.017 (3)	0.008 (3)
C19	0.079 (3)	0.048 (3)	0.084 (3)	−0.022 (3)	−0.002 (3)	−0.003 (3)
C29	0.089 (4)	0.081 (4)	0.082 (4)	−0.009 (3)	−0.025 (3)	0.026 (3)
C5	0.095 (4)	0.110 (5)	0.071 (4)	−0.016 (4)	−0.001 (3)	−0.014 (4)
C4	0.073 (3)	0.115 (5)	0.058 (3)	0.016 (3)	0.010 (3)	0.003 (4)
C3	0.092 (4)	0.062 (3)	0.067 (3)	0.005 (3)	0.023 (3)	0.010 (3)
C28	0.112 (4)	0.071 (4)	0.062 (4)	0.000 (3)	−0.013 (3)	0.001 (3)
C22	0.115 (5)	0.067 (4)	0.068 (3)	0.028 (4)	−0.003 (3)	0.017 (3)

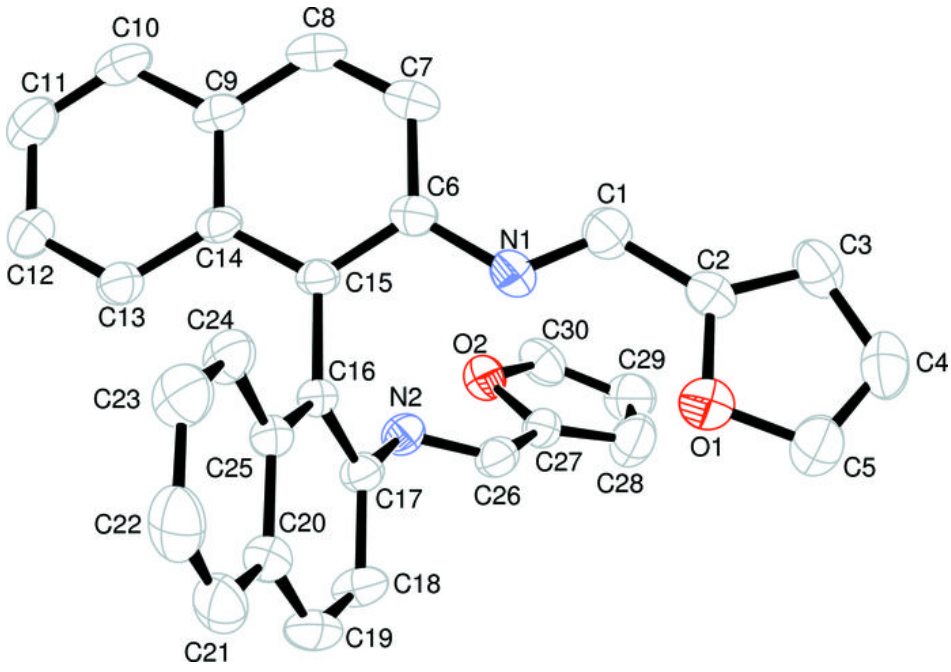
Geometric parameters (Å, °)

C15—C6	1.374 (5)	C26—H26	0.95 (3)
C15—C14	1.434 (5)	C20—C19	1.409 (5)
C15—C16	1.488 (5)	C20—C21	1.413 (6)
O2—C27	1.363 (4)	C8—C7	1.366 (5)
O2—C30	1.373 (5)	C8—H8	0.9300
C14—C9	1.395 (5)	C13—H13	0.9300
C14—C13	1.421 (5)	C24—C23	1.357 (5)
N2—C26	1.268 (4)	C24—H24	0.9300
N2—C17	1.421 (4)	C1—H1	1.09 (4)
C16—C17	1.374 (4)	C7—H7	0.9300
C16—C25	1.420 (5)	C30—C29	1.320 (6)
C6—C7	1.418 (5)	C30—H30	1.04 (4)
C6—N1	1.420 (4)	C11—C10	1.356 (6)
C17—C18	1.410 (5)	C11—H11	0.9300
N1—C1	1.264 (5)	C10—H10	0.9300
O1—C2	1.354 (5)	C21—C22	1.359 (6)
O1—C5	1.370 (5)	C21—H21	0.9300
C9—C8	1.415 (5)	C23—C22	1.385 (6)
C9—C10	1.416 (5)	C23—H23	0.9300
C18—C19	1.361 (5)	C19—H19	0.9300
C18—H18	0.9300	C29—C28	1.392 (6)
C27—C28	1.339 (5)	C29—H29	0.95 (4)
C27—C26	1.431 (5)	C5—C4	1.308 (7)
C12—C13	1.357 (5)	C5—H5	1.08 (4)
C12—C11	1.394 (5)	C4—C3	1.416 (7)
C12—H12	0.9300	C4—H4	0.92 (4)
C25—C24	1.407 (5)	C3—H3	0.94 (4)
C25—C20	1.418 (5)	C28—H28	0.93 (4)
C2—C3	1.348 (5)	C22—H22	0.9300
C2—C1	1.445 (5)		

C6—C15—C14	118.8 (4)	C12—C13—H13	119.6
C6—C15—C16	120.6 (3)	C14—C13—H13	119.6
C14—C15—C16	120.6 (4)	C23—C24—C25	121.4 (4)
C27—O2—C30	106.2 (3)	C23—C24—H24	119.3
C9—C14—C13	118.0 (4)	C25—C24—H24	119.3
C9—C14—C15	120.4 (4)	N1—C1—C2	121.8 (4)
C13—C14—C15	121.6 (4)	N1—C1—H1	122 (2)
C26—N2—C17	117.9 (3)	C2—C1—H1	115.8 (19)
C17—C16—C25	119.3 (3)	C8—C7—C6	120.5 (4)
C17—C16—C15	120.8 (3)	C8—C7—H7	119.8
C25—C16—C15	119.9 (3)	C6—C7—H7	119.8
C15—C6—C7	120.6 (4)	C29—C30—O2	110.1 (5)
C15—C6—N1	116.2 (4)	C29—C30—H30	136 (2)
C7—C6—N1	123.2 (4)	O2—C30—H30	114 (2)
C16—C17—C18	120.6 (4)	C10—C11—C12	120.2 (4)
C16—C17—N2	119.3 (3)	C10—C11—H11	119.9
C18—C17—N2	120.0 (3)	C12—C11—H11	119.9
C1—N1—C6	120.5 (4)	C11—C10—C9	120.2 (4)
C2—O1—C5	106.8 (4)	C11—C10—H10	119.9
C14—C9—C8	119.1 (4)	C9—C10—H10	119.9
C14—C9—C10	120.1 (4)	C22—C21—C20	120.9 (5)
C8—C9—C10	120.9 (4)	C22—C21—H21	119.6
C19—C18—C17	119.8 (4)	C20—C21—H21	119.6
C19—C18—H18	120.1	C24—C23—C22	121.2 (4)
C17—C18—H18	120.1	C24—C23—H23	119.4
C28—C27—O2	108.8 (4)	C22—C23—H23	119.4
C28—C27—C26	133.2 (5)	C18—C19—C20	122.4 (4)
O2—C27—C26	118.0 (4)	C18—C19—H19	118.8
C13—C12—C11	120.9 (4)	C20—C19—H19	118.8
C13—C12—H12	119.6	C30—C29—C28	106.9 (5)
C11—C12—H12	119.6	C30—C29—H29	123 (3)
C24—C25—C20	117.4 (4)	C28—C29—H29	130 (3)
C24—C25—C16	121.9 (4)	C4—C5—O1	110.2 (5)
C20—C25—C16	120.6 (4)	C4—C5—H5	142 (2)
C3—C2—O1	109.3 (4)	O1—C5—H5	107 (2)
C3—C2—C1	131.9 (5)	C5—C4—C3	107.3 (5)
O1—C2—C1	118.7 (4)	C5—C4—H4	127 (3)
N2—C26—C27	124.5 (4)	C3—C4—H4	126 (3)
N2—C26—H26	122 (2)	C2—C3—C4	106.4 (4)
C27—C26—H26	113 (2)	C2—C3—H3	123 (3)
C19—C20—C21	123.4 (4)	C4—C3—H3	130 (3)
C19—C20—C25	117.2 (4)	C27—C28—C29	107.9 (5)
C21—C20—C25	119.4 (4)	C27—C28—H28	123 (3)
C7—C8—C9	120.5 (4)	C29—C28—H28	129 (3)
C7—C8—H8	119.7	C21—C22—C23	119.7 (5)
C9—C8—H8	119.7	C21—C22—H22	120.2
C12—C13—C14	120.7 (4)	C23—C22—H22	120.2
C6—C15—C14—C9	−2.4 (5)	C16—C25—C20—C19	0.8 (5)
C16—C15—C14—C9	176.0 (3)	C24—C25—C20—C21	0.2 (5)

C6—C15—C14—C13	177.8 (3)	C16—C25—C20—C21	178.3 (4)
C16—C15—C14—C13	−3.8 (5)	C14—C9—C8—C7	0.3 (6)
C6—C15—C16—C17	−76.0 (5)	C10—C9—C8—C7	−179.5 (4)
C14—C15—C16—C17	105.6 (4)	C11—C12—C13—C14	−1.2 (6)
C6—C15—C16—C25	101.2 (4)	C9—C14—C13—C12	0.3 (5)
C14—C15—C16—C25	−77.2 (4)	C15—C14—C13—C12	−179.9 (4)
C14—C15—C6—C7	3.3 (5)	C20—C25—C24—C23	0.3 (6)
C16—C15—C6—C7	−175.1 (4)	C16—C25—C24—C23	−177.8 (4)
C14—C15—C6—N1	−178.1 (3)	C6—N1—C1—C2	−175.2 (4)
C16—C15—C6—N1	3.5 (5)	C3—C2—C1—N1	−179.0 (5)
C25—C16—C17—C18	4.0 (5)	O1—C2—C1—N1	5.7 (7)
C15—C16—C17—C18	−178.7 (4)	C9—C8—C7—C6	0.6 (6)
C25—C16—C17—N2	−179.1 (3)	C15—C6—C7—C8	−2.5 (6)
C15—C16—C17—N2	−1.8 (5)	N1—C6—C7—C8	179.1 (4)
C26—N2—C17—C16	124.2 (4)	C27—O2—C30—C29	−0.4 (5)
C26—N2—C17—C18	−58.9 (5)	C13—C12—C11—C10	1.7 (7)
C15—C6—N1—C1	160.8 (4)	C12—C11—C10—C9	−1.3 (6)
C7—C6—N1—C1	−20.7 (6)	C14—C9—C10—C11	0.4 (6)
C13—C14—C9—C8	−179.6 (3)	C8—C9—C10—C11	−179.9 (4)
C15—C14—C9—C8	0.6 (5)	C19—C20—C21—C22	177.0 (4)
C13—C14—C9—C10	0.1 (5)	C25—C20—C21—C22	−0.3 (6)
C15—C14—C9—C10	−179.6 (3)	C25—C24—C23—C22	−0.7 (7)
C16—C17—C18—C19	−0.6 (6)	C17—C18—C19—C20	−2.8 (6)
N2—C17—C18—C19	−177.5 (4)	C21—C20—C19—C18	−174.6 (4)
C30—O2—C27—C28	0.6 (5)	C25—C20—C19—C18	2.7 (6)
C30—O2—C27—C26	179.4 (3)	O2—C30—C29—C28	0.1 (6)
C17—C16—C25—C24	173.9 (3)	C2—O1—C5—C4	−1.1 (6)
C15—C16—C25—C24	−3.4 (5)	O1—C5—C4—C3	0.5 (7)
C17—C16—C25—C20	−4.1 (5)	O1—C2—C3—C4	−0.9 (5)
C15—C16—C25—C20	178.6 (3)	C1—C2—C3—C4	−176.6 (5)
C5—O1—C2—C3	1.2 (5)	C5—C4—C3—C2	0.2 (6)
C5—O1—C2—C1	177.5 (4)	O2—C27—C28—C29	−0.5 (6)
C17—N2—C26—C27	178.6 (3)	C26—C27—C28—C29	−179.1 (4)
C28—C27—C26—N2	177.2 (5)	C30—C29—C28—C27	0.2 (6)
O2—C27—C26—N2	−1.4 (6)	C20—C21—C22—C23	−0.1 (7)
C24—C25—C20—C19	−177.3 (4)	C24—C23—C22—C21	0.6 (7)

Fig. 1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